Lab8 Aseem Shaikh

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1 Lab 8: Cluster Analysis

2 Report by: Aseem Shaikh - 3177031

3 Introduction:

In this assignment, you will perform clustering analysis on three datasets, each containing two features. First we will perform a data analysis and then perform K-means Clustering on Dataset 1. Use silhouette analysis to determine the optimal number of clusters. Generate and display a dendrogram for the agglomerative hierarchical clustering algorithm, cut at the level of optimal k clusters determined by k-means clustering. Part 2 perform agglomerative hierarchical clustering on Dataset 1, Dataset 2, and Dataset 3 using four different linkage types: single, average, complete, and ward.

4 Import Libraries

[ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.cm as cm
import seaborn as sns
from sklearn.cluster import KMeans, AgglomerativeClustering
from sklearn.metrics import silhouette_score, silhouette_samples
from scipy.cluster.hierarchy import dendrogram, linkage
from sklearn.preprocessing import StandardScaler
from sklearn import cluster
import warnings
```

5 Analysis of Dataset 1

[ ]:
```
dataset1_df = pd.read_csv('dataset1.csv', index_col=0)
dataset1_df
```

[ ]:
```
           X1        X2
0  -10.979873 -4.400657
1   -2.351221  4.009736
```

```
2      -6.875246 -4.001372
3      -7.489953 -6.494829
4      -2.760179  5.551214
…          …         …
1495   -8.026246 -9.580244
1496   -8.439024 -1.583618
1497  -10.624320 -3.181229
1498  -10.813260 -4.683275
1499   -9.215925 -8.016927

[1500 rows x 2 columns]
```

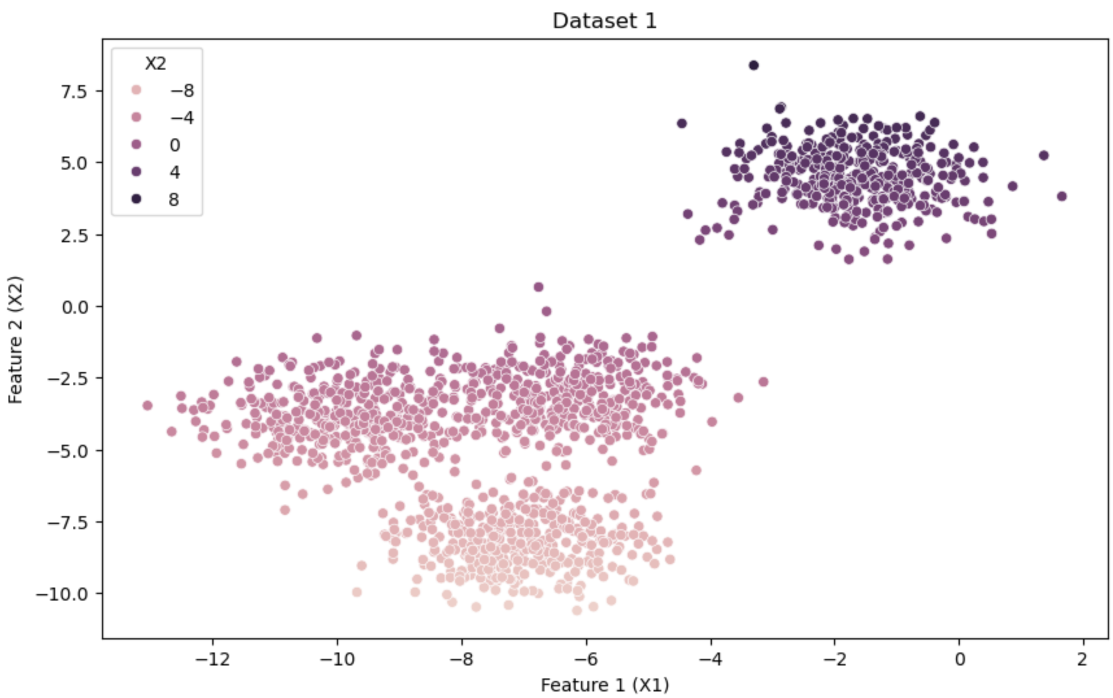
[ ]:
```python
#Other important analysis
print('Dataset 1 Description\n', dataset1_df.describe())
print('\nDataset 1 Info')
dataset1_df.info()
print('\nMissing Values\n', dataset1_df.isna().sum())
```

```
Dataset 1 Description
                  X1           X2
count  1500.000000  1500.000000
mean     -6.232241    -2.682810
std       3.135589     4.661393
min     -13.051477   -10.607120
25%      -8.591130    -6.112957
50%      -6.718760    -3.576407
75%      -4.113229     0.892471
max       1.661519     8.365093

Dataset 1 Info
<class 'pandas.core.frame.DataFrame'>
Index: 1500 entries, 0 to 1499
Data columns (total 2 columns):
 #   Column  Non-Null Count  Dtype
---  ------  --------------  -----
 0   X1      1500 non-null   float64
 1   X2      1500 non-null   float64
dtypes: float64(2)
memory usage: 35.2 KB

Missing Values
 X1    0
X2    0
dtype: int64
```

6 Plotting

[ ]:
```
# Scatter Plot
plt.figure(figsize=(10, 6))
scatter_plot = sns.scatterplot(data=dataset1_df, x='X1', y='X2', hue='X2')
scatter_plot.set_title('Dataset 1')
scatter_plot.set_xlabel('Feature 1 (X1)')
scatter_plot.set_ylabel('Feature 2 (X2)')
```

[ ]:
```
Text(0, 0.5, 'Feature 2 (X2)')
```



It looks like this dataset has 3 clusters.

7 k-Mean Clustering

[ ]:
```
# Initialize KMeans with an arbitrary number of clusters
kmeans = KMeans(n_clusters=3, random_state=42)

# Fit KMeans model to the data
kmeans.fit(dataset1_df)

# Get cluster labels
cluster_labels = kmeans.labels_
silhouette =  silhouette_score(dataset1_df,cluster_labels)
```

```python
print(f'KMeans with an arbitrary number of clusters 3 is {silhouette}')
```

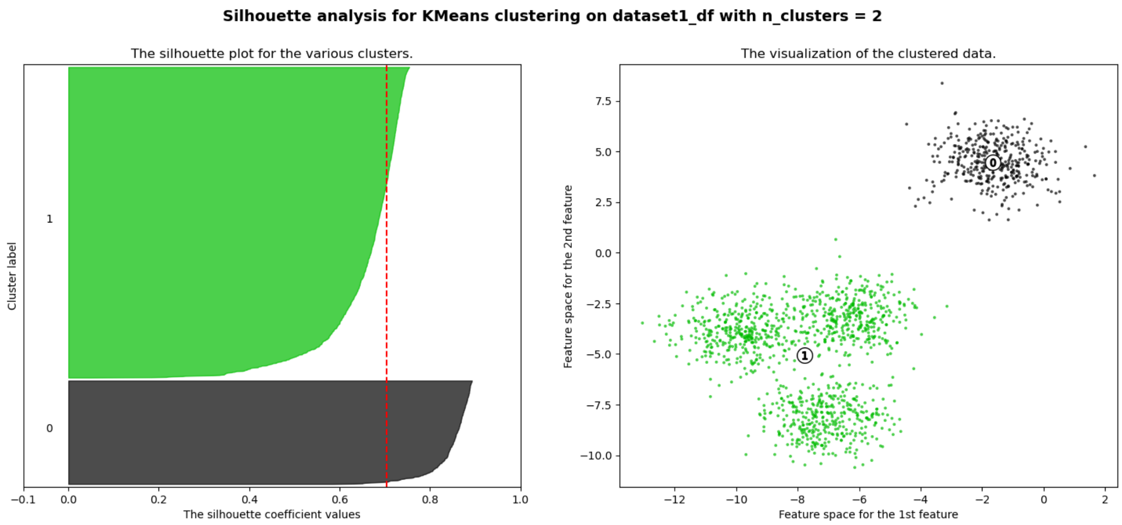
```
KMeans with an arbitrary number of clusters 3 is 0.596962510586324
```

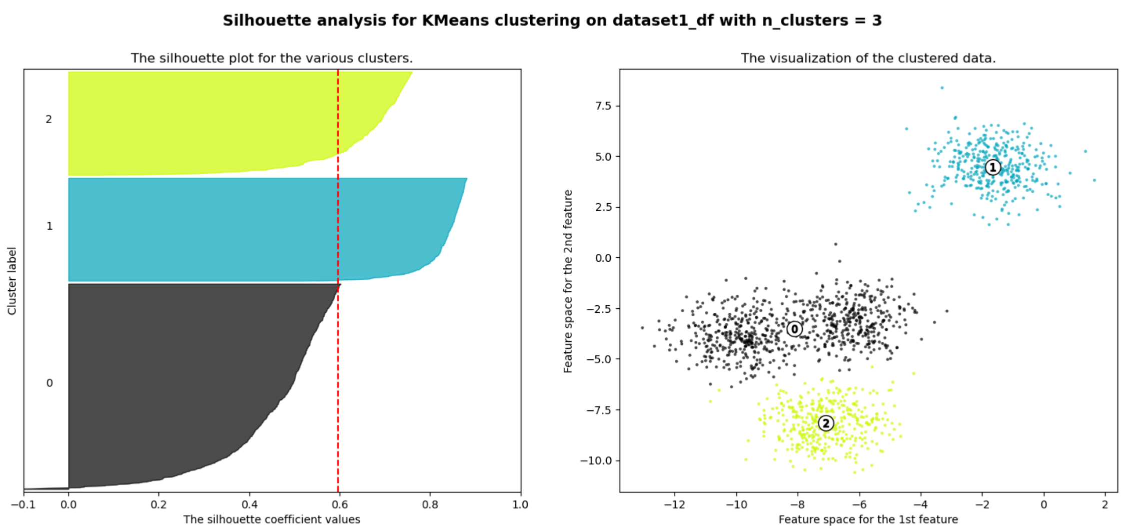
[ ]:
```python
#silhouette analysis using k-mean clustering by testing multiple clusters
silhouette_scores = []

# Defining the range of clusters to analyze
range_n_clusters = range(2, 11)

for n_clusters in range_n_clusters:
    # Create a subplot with 1 row and 2 columns
    fig, (ax1, ax2) = plt.subplots(1, 2)
    fig.set_size_inches(18, 7)

    # The 1st subplot is the silhouette plot
    ax1.set_xlim([-0.1, 1])
    ax1.set_ylim([0, len(dataset1_df) + (n_clusters + 1) * 10])

    # Initialize the KMeans clusterer with n_clusters value
    clusterer = KMeans(n_clusters=n_clusters, random_state=42)
    cluster_labels = clusterer.fit_predict(dataset1_df)

    # Calculate the average silhouette score
    silhouette_avg = silhouette_score(dataset1_df, cluster_labels)
    silhouette_scores.append(silhouette_avg)
    print(f"For n_clusters = {n_clusters}, the average silhouette_score is :␣
↪{silhouette_avg}")

    # Compute the silhouette scores for each sample
    sample_silhouette_values = silhouette_samples(dataset1_df, cluster_labels)

    y_lower = 10
    for i in range(n_clusters):
        # Aggregate and sort silhouette scores for samples belonging to cluster␣
↪i
        ith_cluster_silhouette_values = sample_silhouette_values[cluster_labels␣
↪== i]
        ith_cluster_silhouette_values.sort()

        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.nipy_spectral(float(i) / n_clusters)
        ax1.fill_betweenx(np.arange(y_lower, y_upper), 0,␣
↪ith_cluster_silhouette_values,
                          facecolor=color, edgecolor=color, alpha=0.7)
```

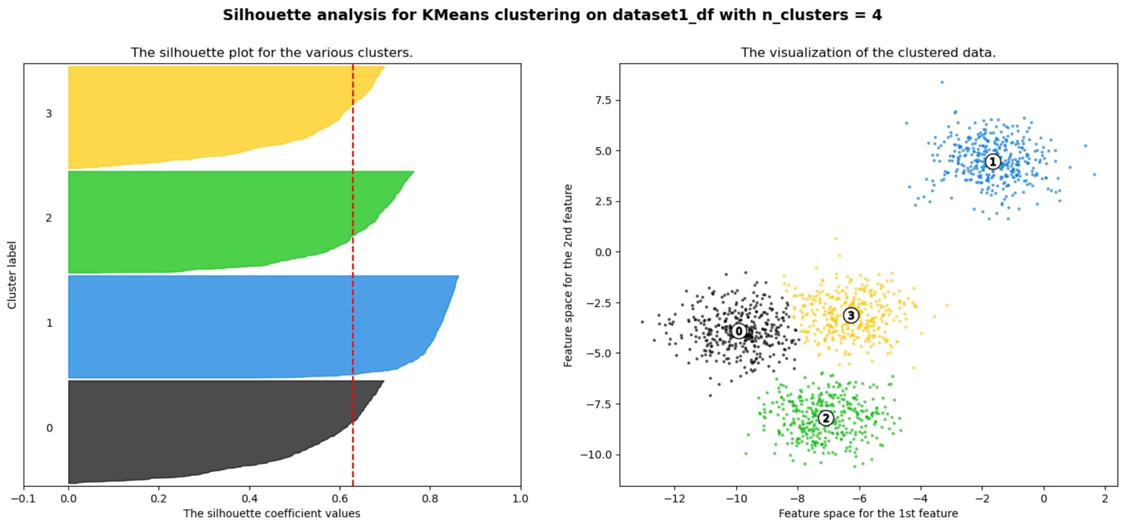
```
        # Label silhouette plots with cluster numbers
        ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

        # Compute the new y_lower for next plot
        y_lower = y_upper + 10  # 10 for the 0 samples

    ax1.set_title("The silhouette plot for the various clusters.")
    ax1.set_xlabel("The silhouette coefficient values")
    ax1.set_ylabel("Cluster label")

    # The vertical line for average silhouette score of all the values
    ax1.axvline(x=silhouette_avg, color="red", linestyle="--")

    ax1.set_yticks([])  # Clear the yaxis labels / ticks
    ax1.set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])

    # 2nd Plot showing the actual clusters formed
    colors = cm.nipy_spectral(cluster_labels.astype(float) / n_clusters)
    ax2.scatter(dataset1_df.iloc[:, 0], dataset1_df.iloc[:, 1], marker=".", s=30, lw=0, alpha=0.7,
                c=colors, edgecolor="k")

    # Labeling the clusters
    centers = clusterer.cluster_centers_
    # Draw white circles at cluster centers
    ax2.scatter(centers[:, 0], centers[:, 1], marker="o", c="white", alpha=1, s=200, edgecolor="k")

    for i, c in enumerate(centers):
        ax2.scatter(c[0], c[1], marker="$%d$" % i, alpha=1, s=50, edgecolor="k")

    ax2.set_title("The visualization of the clustered data.")
    ax2.set_xlabel("Feature space for the 1st feature")
    ax2.set_ylabel("Feature space for the 2nd feature")

    plt.suptitle(f"Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = {n_clusters}",
                 fontsize=14, fontweight="bold")

plt.show()

# Plotting silhouette scores
plt.plot(range(2, 11), silhouette_scores, marker='o')
plt.xlabel('Number of clusters (k)')
plt.ylabel('Silhouette score')
plt.title('Silhouette Analysis for KMeans Clustering')
```

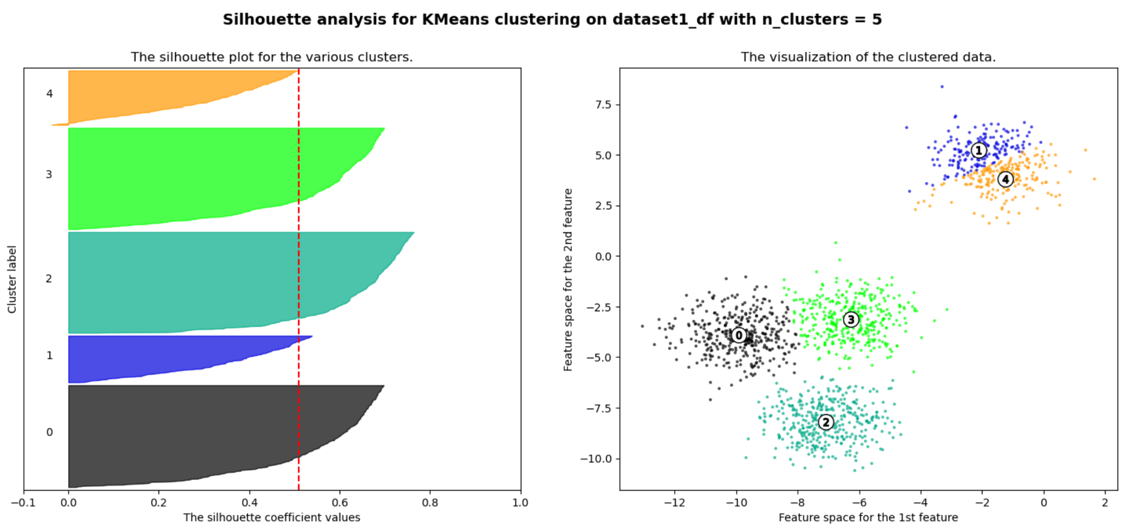
```
plt.show()
```

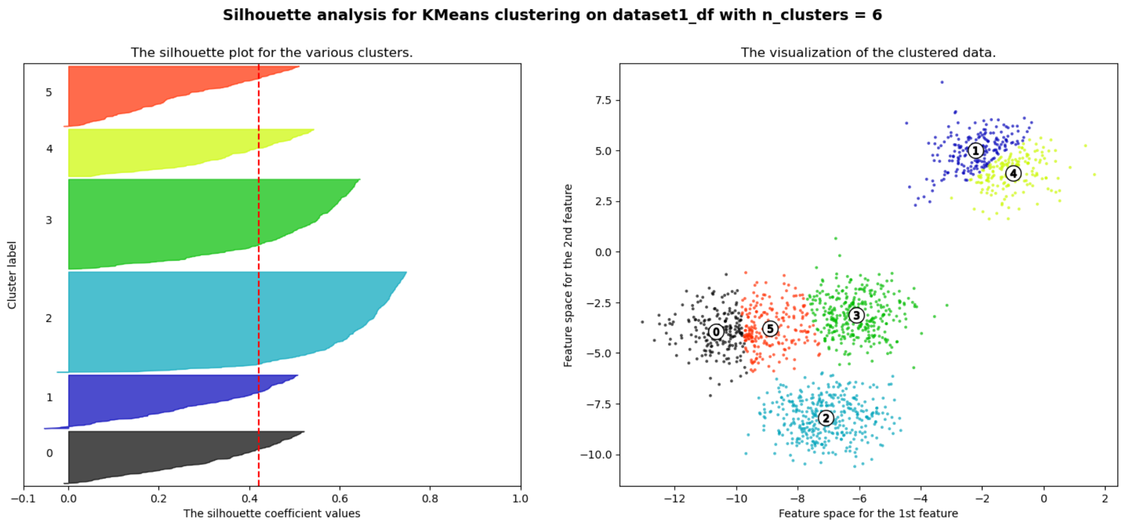
```
For n_clusters = 2, the average silhouette_score is : 0.7047609238906556
For n_clusters = 3, the average silhouette_score is : 0.596962510586324
For n_clusters = 4, the average silhouette_score is : 0.6285541393306969
For n_clusters = 5, the average silhouette_score is : 0.5093017342323468
For n_clusters = 6, the average silhouette_score is : 0.4220494214291892
For n_clusters = 7, the average silhouette_score is : 0.3795995357933134
For n_clusters = 8, the average silhouette_score is : 0.35588751492179077
For n_clusters = 9, the average silhouette_score is : 0.3592911323216888
For n_clusters = 10, the average silhouette_score is : 0.3205635326920583
```

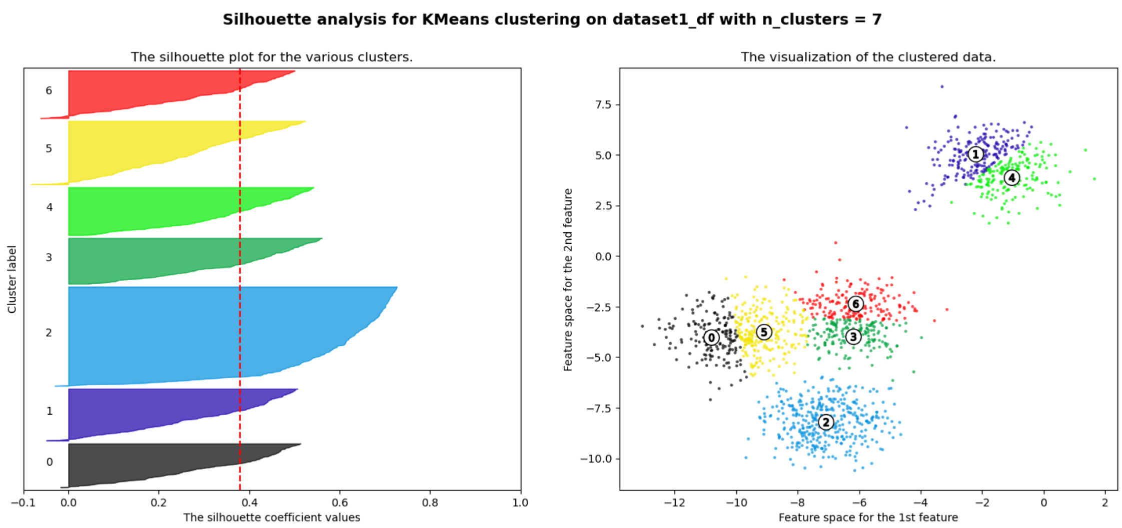


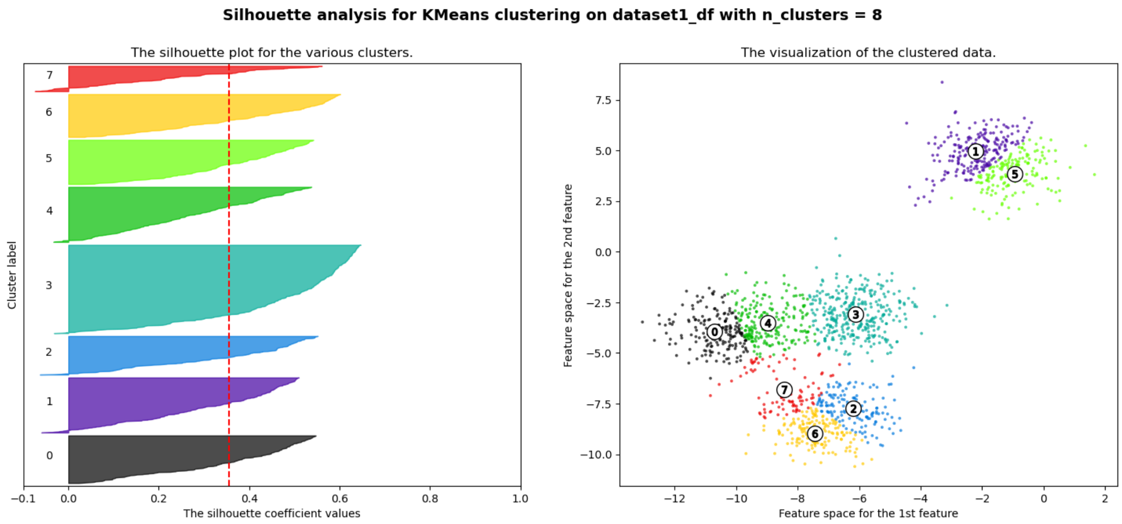


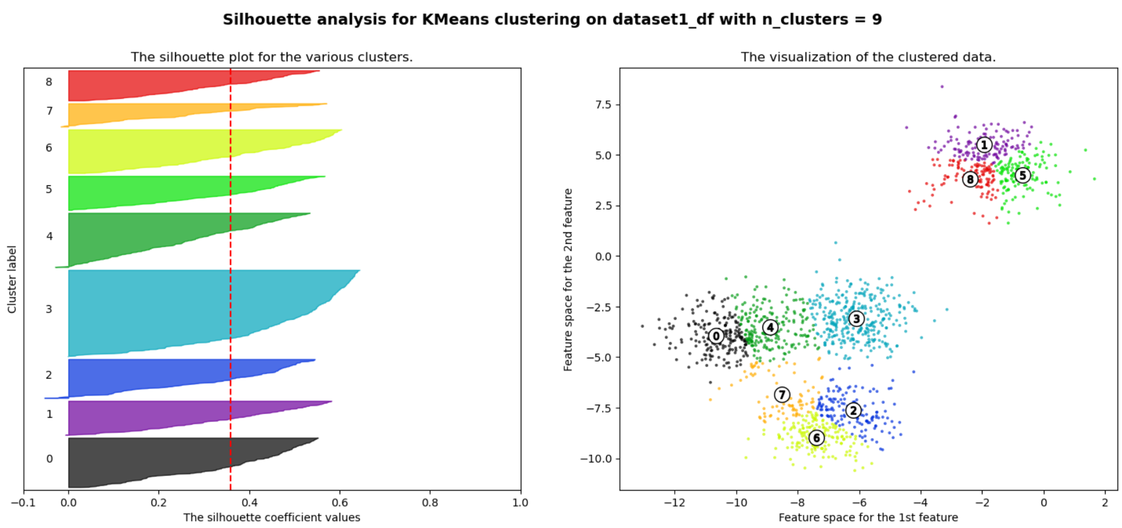

Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 4
The silhouette plot for the various clusters.
Cluster label
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
Feature space for the 1st feature

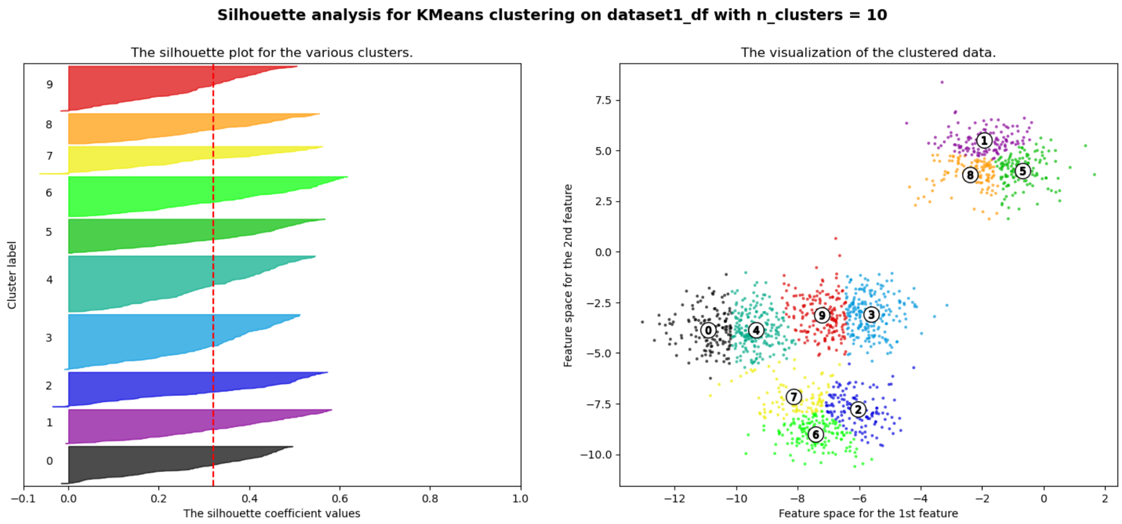

Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 5
The silhouette plot for the various clusters.
Cluster label
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
Feature space for the 1st feature

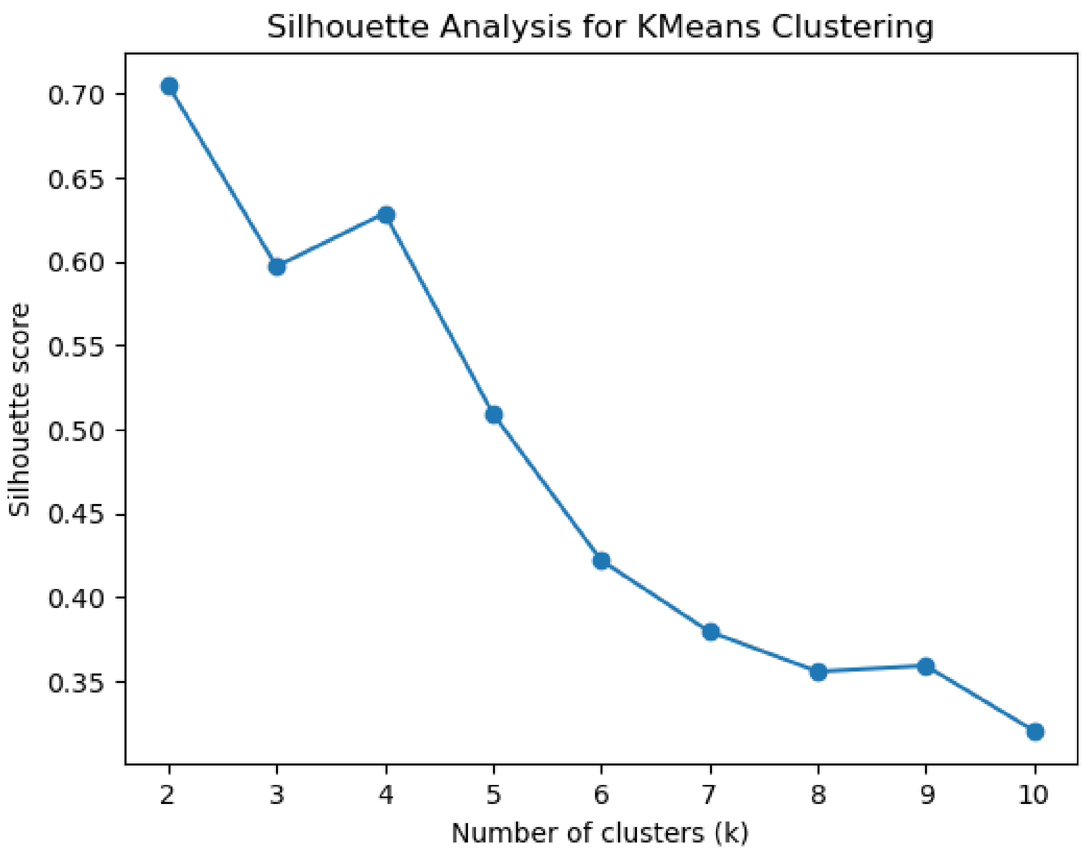

Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 6
The silhouette plot for the various clusters.
Cluster label
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
Feature space for the 1st feature


Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 7
The silhouette plot for the various clusters.
Cluster label
The silhouette coefficient values
The visualization of the clustered data.
Feature space for the 2nd feature
Feature space for the 1st feature


Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 8
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature

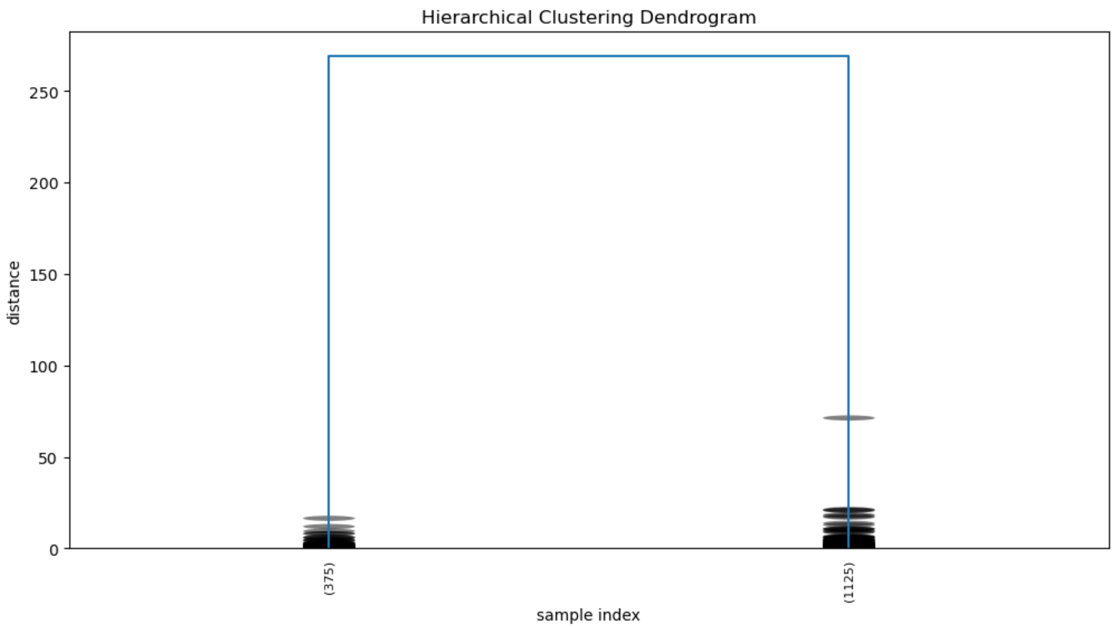

Silhouette analysis for KMeans clustering on dataset1_df with n_clusters = 9
The silhouette plot for the various clusters.
The visualization of the clustered data.
Cluster label
The silhouette coefficient values
Feature space for the 2nd feature
Feature space for the 1st feature





Based on these scores, the highest average silhouette score is for number of clusters = 2 with a score of 0.7047609238906556. Thus, the optimal number of clusters for your dataset based on silhouette analysis is 2.

[ ]:
```python
# Perform hierarchical clustering
optimal_clusters = 2
Z = linkage(dataset1_df, method='ward')

# Plot dendrogram
plt.figure(figsize=(12, 6))
plt.title('Hierarchical Clustering Dendrogram')
plt.xlabel('sample index')
plt.ylabel('distance')
dendrogram(Z, truncate_mode='lastp', p=2, leaf_rotation=90., leaf_font_size=8.,
 ↪show_contracted=True)
plt.show()
```



8 K-Means Clustering Analysis

Results and Silhouette Scores The average silhouette scores for each number of clusters are as follows:

- For clusters = 2 , the average silhouette score is: 0.7047609238906556
- For clusters = 3 , the average silhouette score is: 0.596962510586324
- For clusters = 4 , the average silhouette score is: 0.6285541393306969
- For clusters = 5 , the average silhouette score is: 0.5093017342323468
- For clusters = 6 , the average silhouette score is: 0.4220494214291892
- For clusters = 7 , the average silhouette score is: 0.3795995357933134
- For clusters = 8 , the average silhouette score is: 0.35588751492179077
- For clusters = 9 , the average silhouette score is: 0.3592911323216888

- For clusters = 10 , the average silhouette score is: 0.3205635326920583

Analysis

1. Optimal Number of Clusters:
   - The highest silhouette score is obtained for clusters = 2 with a score of 0.7047609238906556, indicating that the best-defined clusters are achieved when the dataset is divided into 2 clusters.
   - This suggests that the dataset inherently has two distinct groups that are well-separated from each other.
2. Performance with More Clusters:
   - As the number of clusters increases from 2 to 10, the silhouette score generally decreases. This decrease indicates that the quality of the clustering diminishes with more clusters, possibly due to over-segmentation where clusters are forced even when natural groupings do not exist.
   - For example, at clusters = 3 and clusters = 4 , the silhouette scores (0.596962510586324 and 0.6285541393306969, respectively) are still relatively high, suggesting moderately good cluster separation, but not as distinct as for clusters = 2.
3. Cluster Cohesion and Separation:
   - The decreasing silhouette scores indicate that increasing the number of clusters may lead to smaller, less cohesive clusters that are not well-separated from each other.
   - For instance, with clusters = 10 , the silhouette score drops significantly to 0.3205635326920583, highlighting poor clustering where samples might be ambiguously assigned to clusters.

Conclusion The silhouette analysis suggests that the optimal number of clusters for the given dataset is 2. This is based on the highest average silhouette score obtained for clusters = 2. Increasing the number of clusters beyond this point leads to a decrease in clustering quality, as indicated by the declining silhouette scores.

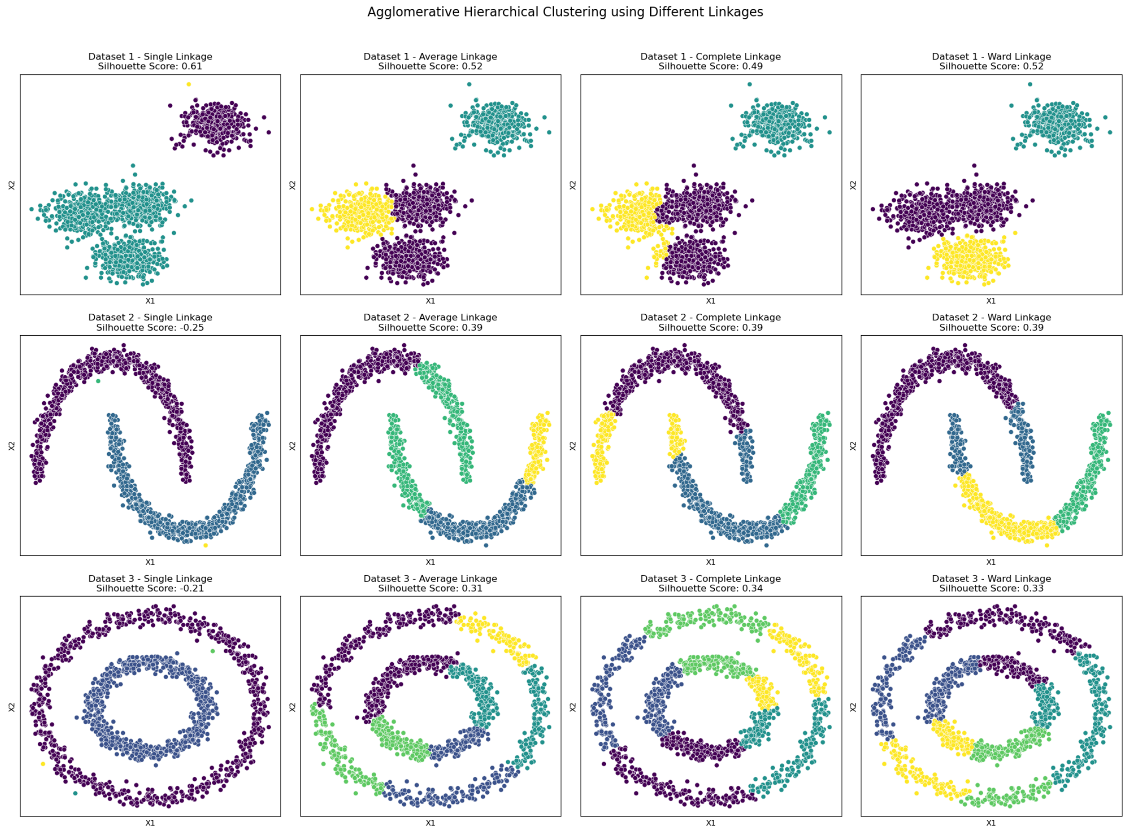
This analysis provides a quantitative basis for choosing the number of clusters in K-Means clustering, ensuring that the chosen clusters are both meaningful and well-separated.

9 Agglomerative hierarchical clustering

[ ]:
```
dataset2_df  = pd.read_csv("dataset2.csv", index_col= 0)
dataset3_df  = pd.read_csv("dataset3.csv", index_col= 0)

# Convert DataFrames to numpy arrays
dataset1 = dataset1_df.values
dataset2 = dataset2_df.values
dataset3 = dataset3_df.values

datasets_list = [dataset1, dataset2, dataset3]
dataset_names = ["Dataset 1", "Dataset 2", "Dataset 3"]

# Modify these based on the appropriate number of clusters for each dataset
```

```
n_clusters_list = [3, 4, 5 , 6, 7, 8]
```

[ ]:
```
# Set up the figure and axes
fig, axes = plt.subplots(len(datasets_list), 4, figsize=(20, 15))
fig.suptitle('Agglomerative Hierarchical Clustering using Different Linkages',␣
↪fontsize=16)

# Linkage methods
linkages = ['single', 'average', 'complete', 'ward']
linkage_names = ['Single', 'Average', 'Complete', 'Ward']

for i, (dataset, n_clusters) in enumerate(zip(datasets_list, n_clusters_list)):
    X = dataset
    X = StandardScaler().fit_transform(X)

    for j, (linkage, linkage_name) in enumerate(zip(linkages, linkage_names)):
        # Perform agglomerative clustering
        algorithm = cluster.AgglomerativeClustering(n_clusters=n_clusters,␣
↪linkage=linkage)

        with warnings.catch_warnings():
            warnings.filterwarnings("ignore", message="the number of connected␣
↪components of the connectivity matrix is [0-9]{1,2} > 1. Completing it to␣
↪avoid stopping the tree early.", category=UserWarning)
            algorithm.fit(X)

        labels = algorithm.labels_.astype(int)

        # Plot the results
        ax = axes[i, j]
        silhouette_avg = silhouette_score(X, labels)
        sns.scatterplot(x=X[:, 0], y=X[:, 1], hue=labels, palette='viridis',␣
↪ax=ax, legend=None)
        ax.set_title(f'{dataset_names[i]} - {linkage_name} Linkage\nSilhouette␣
↪Score: {silhouette_avg:.2f}')
        ax.set_xlabel('X1')
        ax.set_ylabel('X2')
        ax.set_xticks([])
        ax.set_yticks([])

plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
```



10 Agglomerative hierarchical cluster Analysis

Agglomerative hierarchical clustering on three different datasets (`dataset1`, `dataset2`, `dataset3`) using four different linkage methods: Single, Average, Complete, and Ward.

10.0.1 Dataset 1

Single Linkage - The clustering forms two distinct groups with a few outliers. - Single linkage tends to form elongated clusters and can be sensitive to noise and outliers.

Average Linkage - The clusters are more compact compared to single linkage. - Average linkage balances the sensitivity to outliers and tends to form clusters of similar size.

Complete Linkage - The clusters are compact and well-separated. - Complete linkage often creates round-shaped clusters and is less sensitive to outliers compared to single linkage.

Ward Linkage - The clustering is very similar to complete linkage with compact and well-separated clusters. - Ward linkage minimizes the variance within clusters, often resulting in more spherical clusters.

10.0.2 Dataset 2

Single Linkage - The clusters appear to be elongated and poorly separated. - Single linkage can struggle with datasets that have a lot of noise or varying densities.

Average Linkage - The clusters are more balanced and show better separation compared to single linkage. - There are some inconsistencies in cluster shapes, showing the average linkage's balance between sensitivity to outliers and compactness.

Complete Linkage - The clusters are well-separated and relatively compact. - Complete linkage provides a clearer separation of clusters compared to single linkage.

Ward Linkage - The clusters are compact and well-separated, similar to complete linkage. - Ward linkage provides the most distinct and spherical clusters, indicating it handles this dataset well.

10.0.3 Dataset 3

Single Linkage - The clusters are elongated and less distinct, with several overlapping points. - Single linkage is sensitive to noise and may struggle with datasets that have overlapping clusters.

Average Linkage - The clusters are more balanced and distinct compared to single linkage. - Average linkage offers a compromise between sensitivity to outliers and the compactness of clusters.

Complete Linkage - The clusters are well-separated and compact. - Complete linkage provides clear separation and compact clusters, handling the dataset better than single linkage.

Ward Linkage - The clusters are compact and well-separated, similar to complete linkage. - Ward linkage again provides the most distinct and spherical clusters, showing its effectiveness on this dataset.

10.0.4 Conclusion

- Single Linkage: Tends to form elongated clusters, is sensitive to noise and outliers, and may not handle overlapping clusters well.
- Average Linkage: Balances between sensitivity to outliers and compactness, forming more balanced clusters compared to single linkage.
- Complete Linkage: Creates compact and well-separated clusters, less sensitive to noise, and handles overlapping clusters better.
- Ward Linkage: Minimizes variance within clusters, resulting in the most compact and spherical clusters, and often performs best among the four methods for these datasets.